A Generalized Non-Equilibrium Bounce-Back Condition for Multi-Component DdQn Lattice Boltzmann Models with Wetting Applications.

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Abstract will come here...

I. INTRODUCTION

Introduction will come here...

II. KNUDSEN EXPANSION

In diffusive scaling, we get the following for a Knudsen expansion,

$$
\begin{aligned}
f_i^{(0)} &= f_i^{\mathrm{eq},(0)} = w_i \rho^{(0)}, \\
f_i^{(1)} &= f_i^{\mathrm{eq},(1)} = w_i \rho^{(1)} + w_i \rho^{(0)} \frac{\boldsymbol{u}^{(1)} \cdot \boldsymbol{c}_i}{c_s^2}, \\
f_i^{(2)} &= f_i^{\mathrm{eq},(2)} - \frac{\tau}{Sh} \left(c_{i\alpha} \partial_\alpha f_i^{\mathrm{eq},(1)} \right).
\end{aligned} \tag{1}
$$

This gives the non-equilibrium part up to second order in Knudsen number,

$$
\begin{aligned}
f_i^{\mathrm{neq}} = &-\frac{\tau}{Sh} \left(\partial_\alpha \left(w_i c_{i\alpha} \rho^{(1)} \right) + \frac{\rho^{(0)}}{c_s^2} \partial_\alpha \left(w_i c_{i\alpha} c_{i\beta} u_\beta \right) \right) \\
&+ \mathcal{O}\left(Kn^3 \right).
\end{aligned} \tag{2}
$$

We now want to plug this into the equation for the NEBB boundary condition,

$$
\begin{aligned}
f_i^{\mathrm{neq}} &= f_q^{\mathrm{neq}} - \sum_\alpha w_i c_{i\alpha} N_\alpha, \\
N_\alpha &= \frac{1}{\sum_i^{\mathrm{in}} w_i c_{i\alpha}^2} \sum_i^{\mathrm{par}} f_i c_{i\alpha} \equiv C_\alpha \sum_i^{\mathrm{par}} f_i c_{i\alpha}.
\end{aligned} \tag{3}
$$

We now want to add stress corrections,

$$
f_i^{\mathrm{neq}} = f_q^{\mathrm{neq}} - \sum_\alpha w_i c_{i\alpha} N_\alpha - \sum_\mu \sum_\nu w_i c_{i\mu} c_{i\nu} M_{\mu\nu} \tag{4}
$$

The corrections can be found using the expected Navier-Stokes second moment,

$$
\Pi_{\alpha\beta}^{\mathrm{NS}} = -\tau c_s^2 \rho \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha \right) \tag{5}
$$

The velocity gradients can be estimated using finite differences. We now want to ensure the following,

$$
\sum_i c_{i\alpha} c_{i\beta} f_i = \Pi_{\alpha\beta}^{\mathrm{NS}}. \tag{6}
$$

This gives the following tensor equation,

$$
\sum_\mu \sum_\nu Q_{\alpha\beta\mu\nu} M_{\mu\nu} = B_{\alpha\beta} \tag{7}
$$

With the following definitions,

$$
\begin{aligned}
Q_{\alpha\beta\mu\nu} &\equiv -\sum_i^{\mathrm{in}} w_i c_{i\alpha} c_{i\beta} c_{i\mu} c_{i\nu}, \\
A_{\alpha\beta} &\equiv \Pi_{\alpha\beta}^{\mathrm{NS}} - B_{\alpha\beta}, \\
B_{\alpha\beta} &\equiv C_{\alpha\beta} + D_{\alpha\beta} \\
C_{\alpha\beta} &\equiv 2 \sum_i^{\mathrm{out}} c_{i\alpha} c_{i\beta} f_i + \sum_i^{\mathrm{par}} c_{i\alpha} c_{i\beta} f_i \\
&\quad + 2\rho \sum_i^{\mathrm{in}} w_i c_{i\alpha} c_{i\beta} \frac{\boldsymbol{u} \cdot \boldsymbol{c}_i}{c_s^2} \\
D_{\alpha\beta} &\equiv -\sum_\gamma \sum_i^{\mathrm{in}} w_i c_{i\alpha} c_{i\beta} c_{i\gamma} N_\gamma.
\end{aligned} \tag{8}
$$

For a boundary in the yz, xz and xy-planes, Eq. (7) can be solved if we use the D3Q27 stencil. The results are given in Eqns. (11), (12) and (13). Now that we have $M_{\mu\nu}$, we can compute N_α,

$$
\begin{aligned}
\rho u_\alpha &= \sum_i c_{i\alpha} f_i \\
&= \sum_i^{\mathrm{in}} c_{i\alpha} \left(2 w_i \rho \frac{\boldsymbol{u} \cdot \boldsymbol{c}_i}{c_s^2} - \sum_\beta w_i c_{i\beta} N_\beta + m_\alpha \right) \\
&\quad + \sum_i^{\mathrm{par}} c_{i\alpha} f_i + \frac{1}{2} F_\alpha, \\
m_\alpha &= \delta_{n\alpha} B_{\alpha\alpha} + (1 - \delta_{n\alpha}) 2 B_{n\alpha},
\end{aligned} \tag{9}
$$

where the index n indicates the component normal to the boundary. We can now define the following,

$$
\begin{aligned}
D_{nn} &= -N_n / 6, \\
D_{n\alpha} &= -N_\alpha / 18
\end{aligned} \tag{10}
$$

$$\underline{\underline{M}}^{yz} = \begin{pmatrix} -12A_{00} + 9A_{11} + 9A_{22} & -18A_{01} & -18A_{02} \\ -18A_{01} & 9A_{00} - 27A_{11} & -54A_{12} \\ -18A_{02} & -54A_{12} & 9A_{00} - 27A_{22} \end{pmatrix} \tag{11}$$

$$\underline{\underline{M}}^{xz} = \begin{pmatrix} -27A_{00} + 9A_{11} & -18A_{01} & -54A_{02} \\ -18A_{01} & 9A_{00} - 12A_{11} + 9A_{22} & -18A_{12} \\ -54A_{02} & -18A_{12} & 9A_{11} - 27A_{22} \end{pmatrix} \tag{12}$$

$$\underline{\underline{M}}^{xy} = \begin{pmatrix} -27A_{00} + 9A_{22} & -54A_{01} & -18A_{02} \\ -54A_{01} & -27A_{11} + 9A_{22} & -18A_{12} \\ -18A_{02} & -18A_{12} & 9A_{00} + 9A_{11} - 12A_{22} \end{pmatrix} \tag{13}$$